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Perspectives on purpose-driven coupling of energy system models

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ABSTRACT

Energy system models (ESMs) are essential for planning the energy transition and understanding its impacts. However, this transition is inherently complex and cannot always be understood by using just one model. Consequently, efforts linking different model classes are common practice to get insights into the energy system and the different dimensions around it. While existing literature has focused on proposing how such multi-model analyses could be structured, presenting applied cases, or looking into how specific aspects of other knowledge domains are included in energy modelling, a high-level overview of the practice of model coupling with ESMs is lacking. This article puts this practice into perspective by providing an outlook on two aspects: coupling ESM paradigms and model coupling with other knowledge dimensions. Coupling ESMs paradigms have often been used to expand modelling resolution, yet further emphasis should be placed on illustrating contrasting near-optimal system designs and expanding the solution space beyond optimality criteria. Model coupling across knowledge domains is desirable when providing meaningful insights about specific themes, yet, increased complexity of data, multi-model frameworks, and coordination across practices would make an all-encompassing model impractical and calls for purpose-driven model coupling to answer specific questions about the energy transition.

1. Introduction

To mitigate global warming and meet global climate action commitments, a transition towards a decarbonized, clean, and sustainable energy system needs to take place [1]. Abstract representations of the energy system, or energy system models (ESMs), are instrumental for exploring and assessing the impacts of different energy system scenarios that could outline this transition [2]. Moreover, the insights provided by ESMs can support decision-making by providing the means to answer research questions validating existing energy policy, assessing new policy options, setting targets, and driving decisions contributing to the energy transition [3].

A wide range of ESMs exists, possessing distinct technical attributes, methodological considerations, and varying degrees of complexity [4–8]. While ESMs with more complex representations of the energy system are widely used for policy support, modelling efforts often still rely on coupling more than one tool together to complement their capabilities [7]. Model coupling – or linking – can take place by, for example, unilaterally feeding the outputs of one model to another via systematic protocols; iteratively exchanging data between models; creating links in the code to resolve a mathematical problem jointly; or integrating models altogether running as one [9,10].

Different linking categories have been described in the literature [11–13], with Helgesen and Tomasgard [9] synthesizing these categorizations: defining soft-linking as a user-controlled information exchange between models, hard-linking as a formal computer-led transfer of data with shared code from the models, and integrated models as the combination of models running and handling data as one. In the present study, soft-linking is understood as a coordinated purpose-led data exchange between models or modelling algorithms. Among the above, soft-linking is most common across ESM tool developments, while hard-linked and fully integrated models are less frequently observed [7], typically presenting a simplified focus of one of the models over the other [14]. Other than additional model development, hard-linking or fully integrating models present challenges in both the computational effort to solve more complex mathematical constructs and data reconciliation and consistency. This is the case, especially when accounting that data assumptions, model formulations, and outputs can be quite heterogeneous across models [15–20], and across established modelling frameworks to consider (e.g., TIMES [21–42], OSeMOSYS [43–48],

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LEAP [44–46,49–53], EnergyPLAN [30,31,34,49–51,54–102], MESSAGE [11,103], Calliope [104,105], etc.).

Interlinkages also facilitate an integrated modelling approach where complementary features can be used to obtain a cross-cutting representation of the energy system. This also allows parameters exogenous to a single model to be internalized within a model coupling exercise. In turn, this can arguably provide more holistic multidisciplinary insights and realism than what can otherwise be achieved with a single-model approach. Past studies have relied on model linking to expand their scenario analysis by coupling ESMs with life cycle assessment (LCA) [21], behavioral [22], energy demand [43], and economic models [23–27,54], as well as power market models and with other ESMs [28–35,106,107].

Other cross-cutting representations of the energy systems also exist in the form of integrated assessment models (IAMs), which are widely used within the context of climate policy and planning the energy transition. These tools model the complex interactions between the energy, economy, environment, and other Earth systems, thereby providing encompassing representations of transition scenarios and their climate impacts often on a global and macro-regional scale [108]. However, these models present tradeoffs between their wide analytical range and lack of detailed bottom-up resolution of supply technologies and local energy demands [109]. Therefore, IAMs may need to be combined with other support tools like high-resolution bottom-up ESMs to provide a more nuanced view of the energy system [110]. Past studies have focused on linking IAMs to bottom-up models to assess, for example, the impacts of developing gas infrastructure [111] or to have better assessments of variable renewable integration including high spatial, technical and temporal modelling resolutions [36,112].

The trend of model coupling is further highlighted in recent studies that conceptualize multi-model frameworks and their key considerations and apply linked modelling approaches to energy system analyses [10,41,113,114]. In general, these frameworks present different model classes linked together to address questions about the energy transition, representing multiple dimensions of the energy system and its socio-technical context.

For example, Crespo del Granado et al. [113] propose a modelling framework coupling bottom-up ESMs with top-down macro-economic models to broaden the analysis of energy-economic systems and highlight the strengths and limitations of both types of modelling classes. McCullum et al. [114] put forth a framework to link different bottom-up tools, including ESMs, energy demand models, and statistical tools, to represent the impact of end-user behavior on energy demands and the overall system. Similarly, Fattahi et al. [10] propose modelling frameworks consisting of ESMs linked to spatial and economic models to address the existing shortcomings of energy modelling methodologies. Gardumi et al. [42] propose a modelling framework consisting of multiple tools of varying scales and outline the challenges and benefits of such an integrated modelling approach. In the same context, the implications of developing applied multi-model frameworks are put into perspective by Nikas et al. [115], providing an outlook of the challenges and recommended practices and highlighting the need for future actionable research under the context of the European energy transition. Meanwhile, a growing body of work is emerging at the European level, with projects aiming to establish cross-cutting links between ESMs and other model classes to provide answers about different aspects of the energy transition [116–119].

At the same time, recent studies have looked into the broader integration of ESMs and other approaches or with specific aspects of other knowledge domains, although not specifically focusing on the practice of model coupling. For instance, studies have reviewed energy demand modelling and their integration with ESMs [120], the role of geospatial analysis in energy modelling [121–123], the integration of behavioral aspects [124], socio-technical transition theories [125], social and environmental factors in energy modelling [126,127], LCAs [128], and climate and weather models with ESMs [129,130].

However, a high-level overview of the general practice of coupling ESMs, putting into perspective modelling paradigms and coupling dimensions is lacking in the existing literature. Thus, this paper provides a perspective on current research within the growing field of model coupling, looking beyond previous studies which have mostly focused on proposing blueprints for multi-model frameworks or providing specific practical outlooks and cases. Here, a conceptual framework is presented to better understand why coupling across ESM paradigms is needed, then we contextualize coupling of ESMs to models in other knowledge domains and how this aligns within the landscape of the energy transition.

2. Exploring new solution spaces via coupling of ESMs

A recurring theme in energy system analysis is the coupling of ESMs of different scopes among each other. This is often done to reap the benefits of complementary features found across ESMs with different attributes and mathematical formulations. Such features represent different methodological approaches and socio-technical dimensions, and ultimately the modelling outcome of these can lead to representations of vastly different energy system designs and societal configurations.

Two predominant paradigms can be found in energy system modelling: simulation and optimization. Accordingly, these reflect the type of algorithm applied to the underlying mathematical model formulation of a given ESM. Henceforth, a “simulation model” can be broadly understood as a model resolved via a fixed set of rules that seek to replicate the operation of an energy system, where the modeler can heuristically refine parameters and potential systems for analyses. On the other hand, “optimization models” formulate a given energy system as an optimization problem solved by reaching target criteria such as endogenously minimizing or maximizing values for specified parameters or reaching an optimal equilibrium point, under a set of constraints. Lund et al. [131] present these approaches and contrast their theoretical aspects and practical applications; explicitly, they outline how these approaches are used in energy planning to devise scenarios.

The scenarios formulated with simulation models can usually be associated with predictive scenario planning and thus show what can happen in the future under different assumptions without necessarily portraying an optimal solution, and are rather used for openly exploring the impacts of different alternatives and metrics [132]. In contrast, optimization models are more often associated with normative scenario planning, where scenario outputs are prescriptive, showing what should optimally happen under a given set of assumptions, constraints, and optimality criteria [2,131].

Coupling these two approaches can broaden the range of scenarios and analyses that would otherwise be achieved with only a single ESM by enabling complementary features or enhancing an existing framework’s capabilities and providing a consistent and transparent framework to generate different scenario alternatives. For example, complementarity can be seen when linking a long-term spatially explicit cost-optimization capacity expansion ESM with technology-rich bottom-up system modelling [30,31], in spatially explicit power flow optimization models that feed cross-border transmission balances to a simulation model [55,56], or also across energy system optimization models with different formulations and resolution [32].

The linking of simulation and optimization approaches is not limited to coupling pre-established ESMs together. Hybrid models can also emerge from linking these approaches together, taking one model as a black-box calculation engine [133]. This is well illustrated in simulation-based optimization analyses, which often originate from a pre-existing energy system modelling framework being linked to a custom-fitted metaheuristic optimization algorithm. These types of algorithms can be simply described as optimization methods based on a high-level strategy or specific solution-search rationale to find optimality.

Metaheuristic optimizations can be particularly useful due to their ease of applicability with ESMs, ability to solve multi-objective problems with conflicting objectives (e.g., minimizing costs, emissions and/or primary energy supply, maximizing renewable energy shares), and reasonable computation time [134]. Moreover, they allow practitioners to expand the search space that would otherwise be considered for scenario development and potential system designs. Examples of this can be found in simulation-based optimization analyses that coupled ESMs with different algorithms, such as exhaustive search algorithms [57,58], multicriteria decision analysis [59], evolutionary algorithms [60–76] and swarm intelligence algorithms [77–79] for system design and capacity expansion, multi-objective algorithms for transition pathways analysis [80,81], hill-climbing optimization of marginal CO_2 abatement [82,83], and power flow optimization for analyzing cross-border electricity transmission [55,56].

Whether coupling ESMs of different approaches or expanding their modelling approach dimension, it can be said that feature complementarity can be found. As broadly illustrated in Fig. 1, the feasible solution space for one model can be expanded for exploring new system alternatives (which represent both potentially feasible energy system designs and societal configurations), and includes both near-optimal or even contrasting sub-optimal options for a fixed set of optimality criteria and assumptions. This application aligns with recent studies where single energy system optimization models are used to generate a wide range of results representing diverse and vastly different nearly-optimal energy system configurations rather than a single optimal solution [135–141], which can cater for the potentially different perspectives and choices of result-users and decision-makers. In Fig. 1, an analogous exploration of near-optimal alternatives happens in the proximity of a Pareto front, which presents a set of optimal system representations (here, assuming a 2-dimensional view of competing optimization objectives, such as system costs and primary energy supply).

Meanwhile, simulation-based optimization studies typically explore the set of optimal solutions along the Pareto front, focusing on the best compromise solutions as defined by the modeler's criteria, or generating new optimal sets of results by changes in assumptions [64,68,71,75].

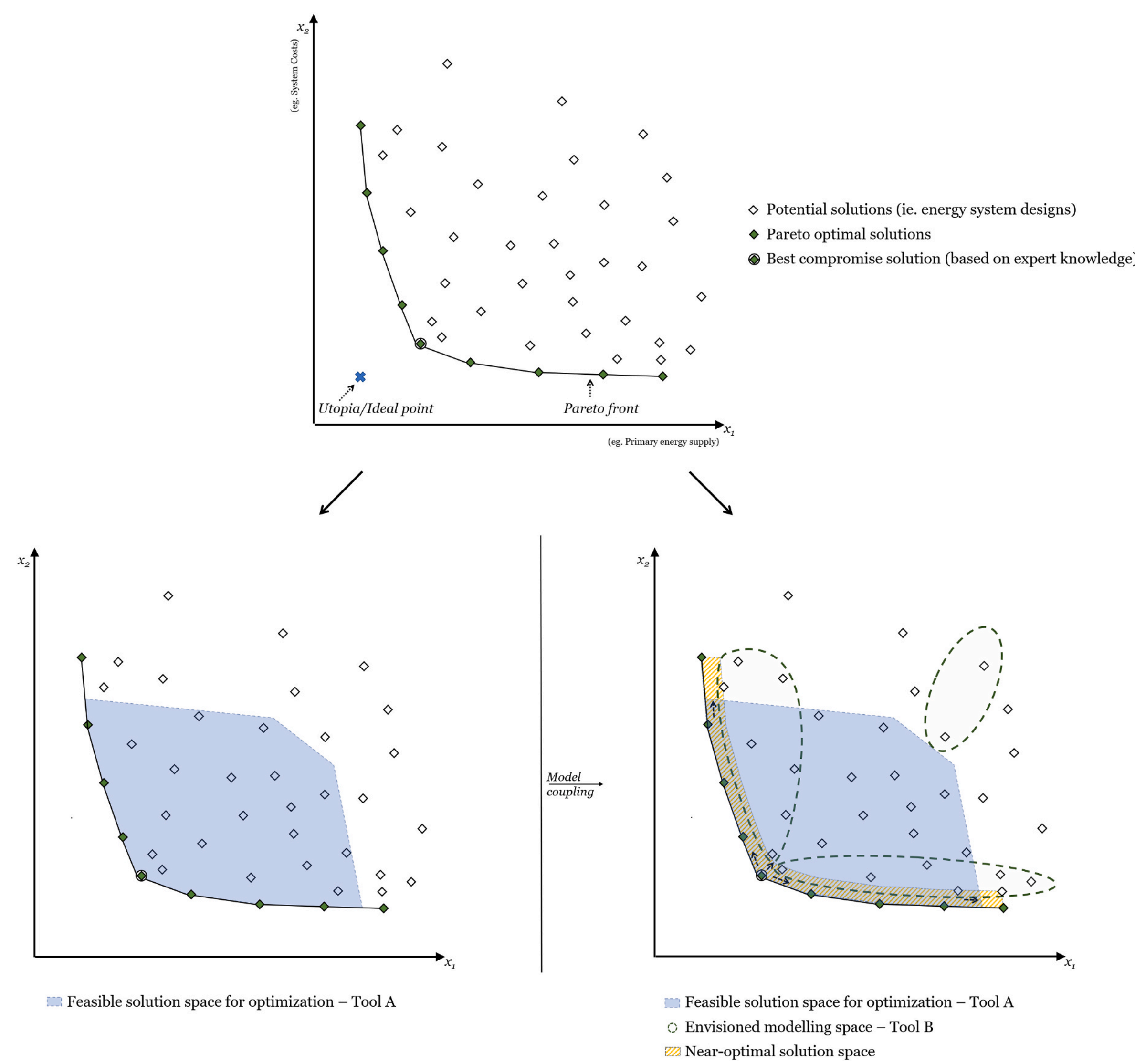

Fig. 1. Conceptual illustrations of the feasible space for energy system designs under a fixed set of assumptions and overlays of the feasible modelling spaces for distinct ESM tools. The axes on the charts represent a simplified 2-d view of competing optimization objectives. The squares represent potentially feasible energy system configurations bounded by the set of Pareto optimal solutions. In the upper chart, the compromise solution (based on modelers' criteria) is depicted as the closest one to the utopia or ideal point, where objectives are at practically unrealizable minima. In the lower-left chart, the shaded area represents the feasible solution space of a given ESM (i.e., Tool A). In the lower right chart, the dashed ovals represent envisioned modelling spaces for a different tool (i.e., Tool B), which overlaps and goes beyond the solution space of Tool A. The top-most right oval encapsulates sub-optimal feasible solutions for the given objectives, while the other ovals cover near-optimal solutions. The cross-shaded area represents the near-optimal solution space, which can be further explored when coupling models.

The diversity of near-optimal options close to the Pareto front, or the compromise solutions, is often not explored to contrast maximally different alternatives. However, studies have contrasted optimal solutions with manually-resolved scenarios from single-model simulations [60,77], showing how these can be found in the near-optimal space. Similarly, coupling ESMs of different scopes could provide a different avenue for exploring said space, or for exploring solutions beyond the feasible scope of one tool by means of the other (in Fig. 1, illustrated by the rightmost oval furthest away from the Pareto front). This is especially relevant when considering computational overhead and solution times of large optimization models [142], which can be complemented with fast resolve times of simulation ESMs [143]. Henceforth, simulation-based optimization studies and coupling of ESMs could further illustrate the diversity of near-optimal and contrasting system designs within the solution space.

3. Coupling knowledge domains and modelling dimensions

Other knowledge domains and their respective modelling classes can provide different perspectives and supplement the capabilities of ESMs to represent parts of real-world systems. This section presents a brief status of linking ESMs across these domains. Then this practice is conceptualized under a multi-level framework.

3.1. Archetypical coupling dimensions

3.1.1. Energy demand

While ESMs are often able to capture both the demand and supply side of the energy system, these models often rely upon demand data as exogenous inputs [7]. Energy demand models are therefore needed to better address questions regarding future demand developments, changes in demand profiles, effects of energy efficiency policy on demands, the location of demands relative to supply sources, and projected changes in the sectoral demands with increased levels of electrification and sector coupling [120].

A classic example of coupling between demand models and ESMs can be found in cases using bottom-up accounting tools (e.g., LEAP [144]) which feed long-term demand projections as inputs to ESMs like OSeMOSYS [43–46,145] or EnergyPLAN [49–53]. Similarly, heating and cooling profiles from buildings can be captured by linking dynamic simulation models with ESMs [84–87]. Specific demand developments can be captured by coupling ESMs with sector-specific models, as has been the case in analyses looking into linking the data from transport sector scenarios [22,88–90]. Although capturing the fine details of the industry sector remains a challenge for ESMs [146], model linkages have been established to bridge this gap in studies analyzing electrification and fuel consumption scenarios in industry [90–92]. Additional linkages in the demand side can also occur when linking to models of consumer behaviors (e.g., consumer patterns, charging profiles of electric vehicles), or with geospatially explicit energy demand analyses.

3.1.2. Geospatial dimension

The spatial dynamics and geographical distribution of the energy system are accounted for to varying degrees in ESMs by considering different modelling resolutions and data aggregations [147]. Matching the level of detail and spatial aggregation of data inputs can be achieved via data processing with geospatial analyses and approaches. Geographic information system (GIS) tools are often used for this purpose to compile and process geo-referenced data which can then be aligned to ESM inputs [148]. Aside from GIS tools, other geostatistical methods can also be applied when aggregating climate and weather data for estimating wind and solar capacity factors at an adequate spatial resolution for these to be linked as inputs to ESMs [122,149].

For example, geospatial analyses have been conducted to estimate the distribution of energy demands, technical potentials of supply, and infrastructure expansion potentials and costs, subsequently linking these into ESMs for national (e.g., Denmark [93,94], Chile [95], the United Kingdom [150], Germany [121]) and European studies [92,96,97]. Moreover, links between GIS and ESMs have been established to iteratively evaluated optimal shares of on- and off-grid electricity generation in rural areas based on estimated levelized costs from the ESMs [47], and for result visualization [37].

3.1.3. Macro-economics

Planning the redesign of future sustainable energy systems has, naturally, broad implications on public finances, economic competitiveness, employment and the economy at large. Therefore, a long tradition exists where top-down macroeconomic models are used to understand the broader socio-economic implications of the energy transition.

Examples of this can be found linking ESMs to econometric models to evaluate economy-wide effects of energy system scenarios [54], or with computable general equilibrium models to capture technological detail and investment flow, and how these affect economic parameters like gross domestic product, commodity prices, sectoral activities and consumption, which in turn result in changes in the energy service demands used by ESMs [14,23–27,103].

3.1.4. Social and behavioral sciences

ESMs typically consider social aspects as exogenous narratives, input assumptions and ex-post discussion of their scenarios, while gathering insights from social sciences on factors such as human behavior, actor heterogeneity, public acceptance, participation and ownership, and societal transformation [126,151]. Nonetheless, these factors can also be integrated into computer modelling and coupled with ESMs. For example, agent-based models (ABMs), which are capable of simulating actor decision-making and interactions, have been used in conjunction with ESMs to integrate EV charging patterns as demand profiles [98], the effects of market uptake of new vehicles [22], and building demand predictions [152,153]. Other standalone applications which could be linked to ESMs include agent-based modelling of capacity investment decisions [154].

System dynamic models – which can represent causal relations of activities and processes – can also be applied in the context of understanding broader societal and behavioral aspects. These have been used as standalone applications to, for example, capture the sociopolitical feasibility of energy transition pathways based on governmental decision-making dynamics, human behavior, and societal change [155–157]. Nonetheless, these aspects which can commonly be associated with the formulation of socio-technical pathways could also stem from other quantification approaches of social drivers and constraints of the diffusion of energy technologies applied to creating energy-related socio-technical narratives, such as those presented by Süsser et al. [158].

3.1.5. Environmental and earth sciences

The environmental effects of the energy transition and the reduction of greenhouse gas (GHG) emissions are core decision drivers in the modelling and policy interface. Indeed, this is reflected in ESMs which often include CO_2 and other GHG emissions in their core modelling capabilities. However, the scope of these calculations is usually limited to only include direct sector-specific emissions from combustion processes.

Therefore, a large body of work has utilized alternative tools to assess the energy-related emissions embedded in upstream processes of the system; namely, applying LCA tools [128]. These often focus on a specific sector or activity, gathering energy and technology mixes ex-post to derive life-cycle emissions and impacts. Examples of this include linking ESMs to LCAs assessing technologies in the electricity supply [38,39,99,100], buildings' renovation rates [159], the use and integration of electric vehicles [101,102], and system impacts when applying power-to-methane [21], as well as other system-wide impact assessment [160–162].

A key challenge of these remains in the accounting of future energy mixes and prospective new life-cycle inventories [163]. At the same time, a broader understanding of material flow models coupled to ESMs needs to be considered further, to assess the needs for rare earth minerals and resources required in the long-term energy scenarios' value chains, and to quantify how circular economy measures (e.g., recycling rates) influence material availability in energy systems [164]. Some of these aspects can partially be addressed by coupling ESMs with IAMs [108], which can include natural resource availability, however, the global scale and broad coverage of IAMs sit in contrast to simpler more targeted models [110]. Nonetheless, when linking ESMs to IAMs an additional interface to climate modelling is enabled, putting aspects of bottom-up energy modelling into perspective with regard to climate change mitigation.

3.2. Representing model coupling from a multi-level perspective

The dynamics of the energy transition include the interplay of a plurality of actors, disciplines, institutions, technologies and radical change. Neither energy systems modelling nor other science domains alone can capture all the aspects of said socio-technical transition [165]. Coordination across models is therefore needed and requires further development and structuration. However, these will be influenced by both model developments stemming from within specific expertise niches and the broad landscape discussions on climate change, energy, policy, geopolitics, grassroots movements and activism.

A multi-level perspective, which provides an analytical framework for socio-technical transitions [166–168], can illustrate how the practice of model coupling and the dynamics across knowledge domains shape the modelling interface in this context. The different levels can be conceptualized under a nested hierarchy, starting at the bottom with novelty and niche areas, in the middle with established configurations or regimes, and at the top with exogenous landscape developments [169, 170]. This is conceptually illustrated in Fig. 2.

In the bottom hierarchy, different domain niches appear, representing the different disciplines and fields of expertise where modelling developments originate. This implies that at this level, modelers work on their own models, with limited external coordination. On the other end, the landscape level includes external mainstay factors such as climate change, sustainable development, global climate action commitments like the Paris Agreement, global trends, national and regional policy, geopolitics, and grassroots activism, all of which exert pressure on the lower levels driving their development and in the long term are also influenced by these. These two levels are connected by an intermediate level, which encapsulates the different pockets of connected niches, and which in turn is pressured by developments in the landscape level.

At the middle level, modelling exercises are conceptualized as different model patchworks and established practices, encapsulating elements stemming from the niches illustrated in Fig. 2, that can generate insight into potential energy transition pathways. Naturally, the structures presented at this level influence each other, drive model developments in the lower individual domains, and can seep through to broader and actionable developments at the landscape level, for instance, guiding long-term energy policy and target setting to reach global climate commitments. This can be exemplified in the current European energy system modelling scene, with projects driving both individual model developments and innovation with multi-model ensembles [42,115–117]. Moreover, some of these patchworks represent deep-rooted modelling practices and interdisciplinarity approaches, with developments of their own vocabulary and standards [171–173]. With increased structuration and model complexity, the idea of striving for an all-encompassing model or building highly coupled multi-model frameworks comes into question. These would require immense degrees of coordination in terms of aligning modelling paradigms, resolution, ontologies, data harmonization, computing power and transparency while keeping up with developments within the niche domains and the timeline and happenings of the energy transition, which also exert further pressure to model developments and the coupling of models to address specific issues. More so, when also

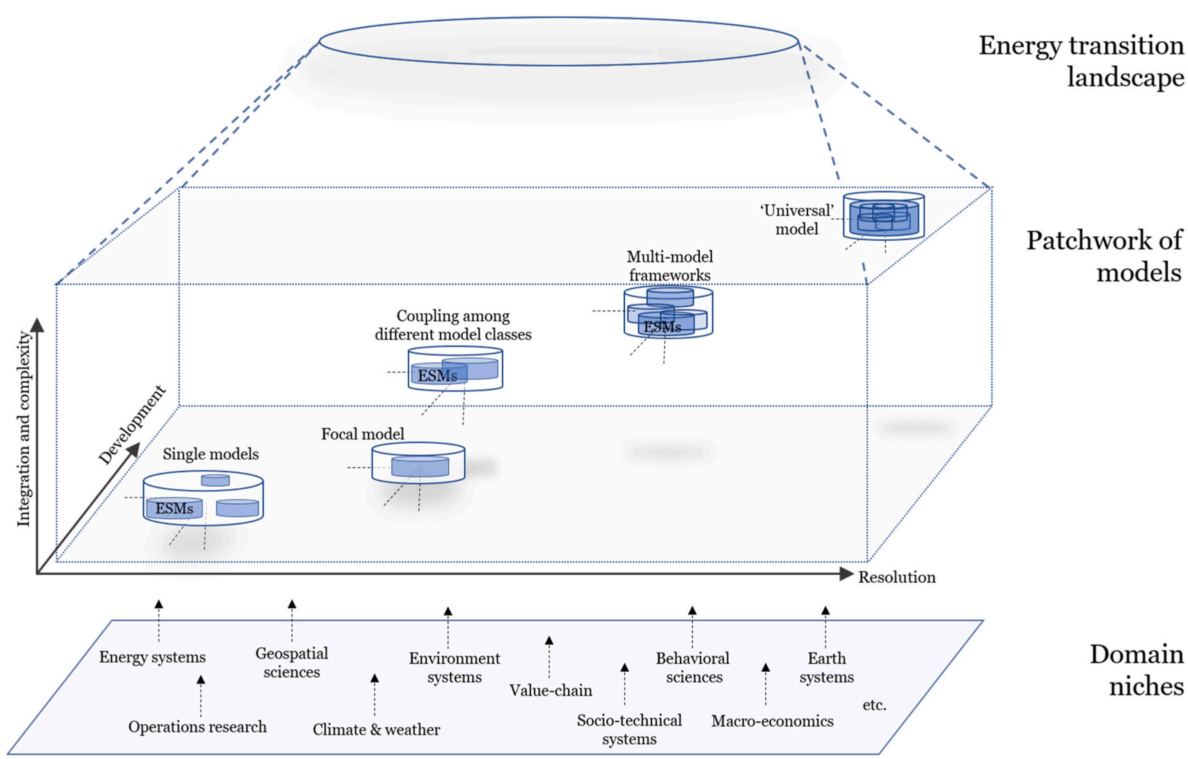

Fig. 2. Conceptual nested hierarchy of modelling dimensions and model coupling showing a multi-level perspective on the emerging practice of model couplings under the context of the energy transition. Inspired by Ref. [170].

aligning additional modelling complexity to the needs and capabilities of both modelers and result-users [174–176], as well as the needs of decision-makers to have timely yet robust insights. Therefore, model coupling should be purpose-driven: designed to address specific research questions, enabling manageable degrees of complexity, resolution, and coordination across knowledge domains, so that it can provide actionable and timely insight for the energy transition.

4. Summary and conclusions

In this perspective, we present the current landscape in the practice of coupling energy system models. Reviewing the current status of coupling ESMs shows that said modelling with multi-model frameworks is becoming ever more prevalent. Model coupling provides multi-dimensional views capable of addressing questions about the potential pathways of the energy transition in a more encompassing manner than what could be achieved with a single model.

Simulation and optimization approaches used by ESMs are commonplace and can provide mutually complementary aspects for analyzing different aspects of the future energy system. This can also be achieved by coupling one model class to optimization algorithms, as is the case in simulation-based optimization modelling. Nonetheless, these have mostly focused on providing a view of the Pareto optimal solutions under different assumptions without exploring near-optimal options with potentially drastically different system designs. This contrast with the growing field of analysis performed with optimization ESMs generating alternatives to explore near-optimal yet maximally different scenarios. Nonetheless, coupling approaches can enable a wider exploration of the solution space than would otherwise be obtained with a single-model approach. This can provide energy planners with more robust scenarios, and consistent scenario design frameworks, that can address not just near-optimality but also the incremental aspects of public planning that might be outside of the scope of certain optimality criteria.

Coupling ESMs with other model classes rooted in other expertise niches allows for a nuanced view of other dimensions to consider beyond only the setup of the energy system itself. In turn, model coupling or even devising multi-model frameworks can be a valid development to improve modelling realism once the tradeoffs in data and modelling uncertainty and additional complexity are weighted. That being said, certain types of archetypical connections present gaps in research. Overall, linkages between ESMs with demand-side models, geospatial models, macroeconomic models, and LCA models seem to have a long-standing presence. However, gaps remain in establishing model links addressing the human and social dimensions, and links to models capable of evaluating upstream value chains of the material flow of resources needed in the future energy transition, as well as the communication of methodological approach, including how and to what extent coupling is performed.

Finally, model coupling should not necessarily strive to be universally comprehensive but rather purpose-driven. That is, addressing specific and meaningful questions that can influence the energy transition landscape while adequately managing complexity, modelling resolution and interdisciplinary coordination.

Credit author statement

Miguel Chang: Conceptualization, Methodology, Formal analysis, Investigation, Writing – original draft, Writing – review & editing. **Jakob Zink Thellufsen:** Conceptualization, Writing – review & editing, Supervision, Project administration. **Henrik Lund:** Conceptualization, Supervision, Writing - review & editing. **Poul Alberg Østergaard:** Writing - review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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